

Issues in Computational Modeling of Biological Systems

Key Features:

- A. Hierarchical (gene-protein-cell-tissue-organ-organism-population...)
- B. Molecular properties are crucial (levels, equilibrium-kinetic-mechanic-transport)
- C. Incomplete data for foreseeable future

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Key Questions:

A. How best to treat hierarchical nature (gene-protein-cell-tissue-organ-organism...)?

1. *Perspective:*

“Bottom-up” (what is a system capable of?)

“Top-Down” (how does a system operate?)

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Key Questions:

A. How best to treat hierarchical nature (gene-protein-cell-tissue-organ-organism...)?

2. *Framework:*

multi-scale models

“modular” models

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Key Questions:

B. Molecular properties are crucial, but how best to treat complex molecular networks:

physico-chemical approach?

electrical circuit approach?

computational algorithm

approach?

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Key Questions:

C. Data will be incomplete for foreseeable future; what types of models will be most useful?

detailed simulations for accessible systems

idealized models for conceptual behavior

“input/output” for elucidation of design principles

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Key Questions:

C. Data will be incomplete for foreseeable future; what types of experimental data are most crucial to seek?

parameter determination

discovery of relationships

effects of property manipulations